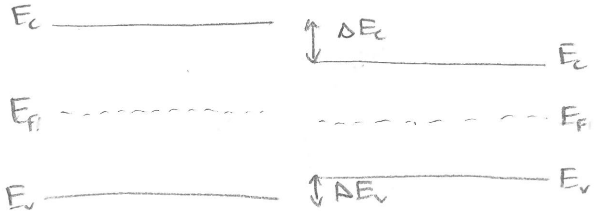
3.1) a.

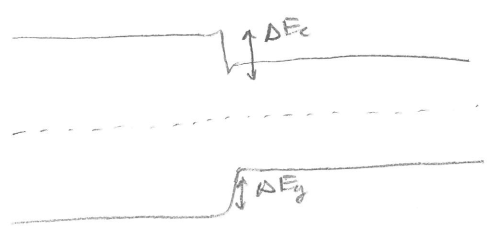
1. If both sides of the junction are intrinsic the Fermi level will be approx in the middle of the gap on each side so:

before



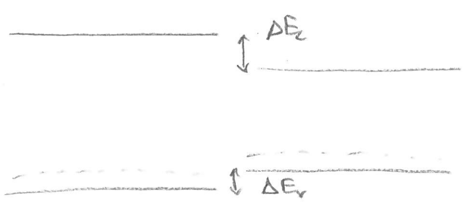
When they come in contact, the bands will bend just slightly, but the main features will be the offsets:

after



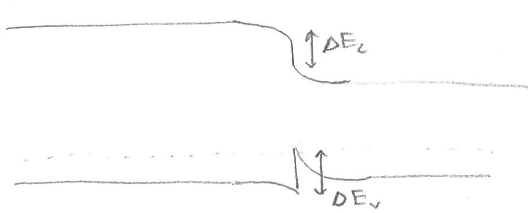
2. Now they are both p doped, so:

before

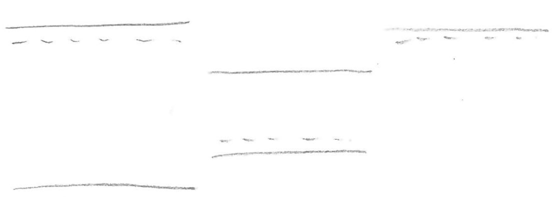


Now there will be some band bending, but it will be small:

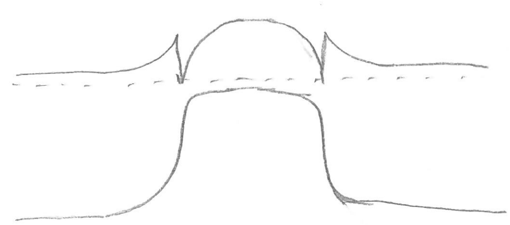
after



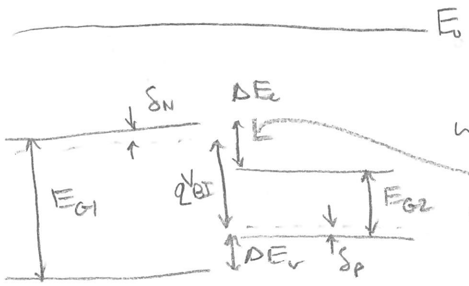
3. before:



after:



4.



The built-in potential is just determined from $E_{FN} - E_{FP}$, which can easily be seen graphically.

Using the values from the paper, $\Delta E_c = 0.23$ eV
$\Delta E_v = 0.15$ eV
$E_{G1} = 1.8$ eV
$E_{G2} = 1.42$ eV

4. (continued) Just from the diagram, then, $qV_{BI} = E_{FN} - E_{FP} = -\delta_N + \Delta E_c + E_{G2} - \delta_p$

δ_N and δ_p come from the doping:

$$\delta_N = kT \ln\left(\frac{N_c}{N_D}\right), \quad \delta_p = kT \ln\left(\frac{N_v}{N_A}\right)$$

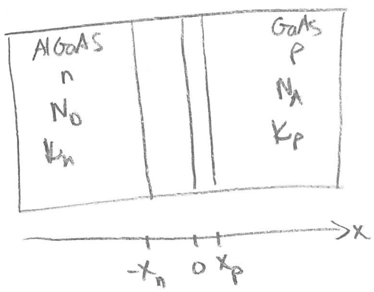
For $Al_{0.6}Ga_{0.4}As$, $N_c = 6.52 \times 10^{17}$ cm^{-3}

GaAs, $N_v = 9 \times 10^{18}$ cm^{-3}

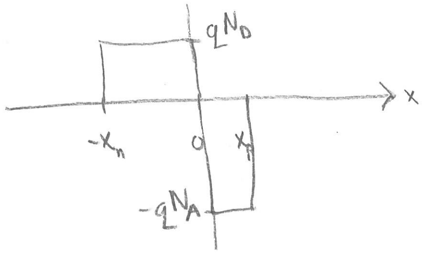
So with these #s, $\delta_N = 30.4$ meV, $\delta_p = -2.7$ meV

So $V_{BI} = \dfrac{\Delta E_c + E_{G2} - \delta_N - \delta_p}{q} = \boxed{1.62\text{ V}}$ in magnitude

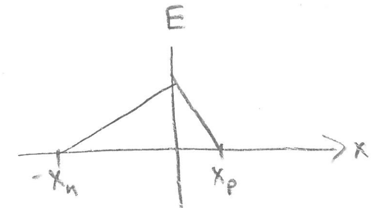
5. The system looks like:



Using the depletion approx, ρ looks like:



Gauss's Law: $\dfrac{dE}{dx} = \dfrac{\rho}{K\varepsilon_0}$



Integrating to get E: $E(x) = \begin{cases} \dfrac{qN_D}{K_n\varepsilon_0}(x + x_n), & -x_n < x < 0 \\ \dfrac{-qN_A}{K_p\varepsilon_0}(x - x_p), & 0 < x < x_p \end{cases}$

Integrating again to get V; with $V(x < -x_n) = 0$: $V(x) = -\int E\,dx'$ and $V(x_p) = V_{BI}$

$$V(x) = \begin{cases} -\dfrac{qN_D}{2K_N\varepsilon_0}(x + x_n)^2 & -x_n < x < 0 \\ \dfrac{qN_A}{2K_p\varepsilon_0}(x - x_p)^2 - V_{BI} & 0 < x < x_p \end{cases}$$

This is negative because the p side is at positive x.

These must be = at $x = 0$, so:

① $$-\frac{qN_D}{2K_N\varepsilon_0}x_n^2 = \frac{qN_A}{2K_p\varepsilon_0}x_p^2 - V_{BI}$$

Finally, charge conservation requires $N_D x_n = N_A x_p$ ②

Solving ① and ② for x_n and x_p gives:

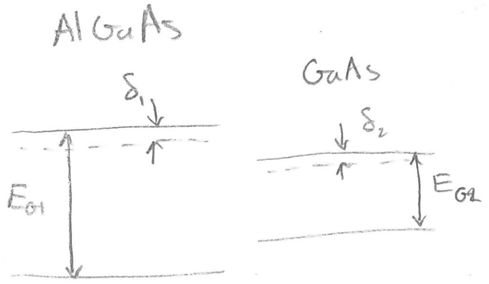
$$x_n = \sqrt{\frac{2K_pK_n\varepsilon_0 N_A V_{BI}}{qN_D(N_A K_p + N_D K_N)}}, \quad x_p = \sqrt{\frac{2K_pK_N\varepsilon_0 N_D V_{BI}}{qN_A(N_A K_p + N_D K_N)}} \rightarrow \boxed{x_n = 97.4\text{ nm},\ x_p = 1.95\text{ nm}}$$

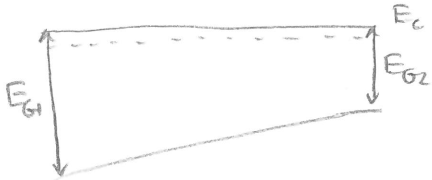
Plugging in to get $E(0^-)$, $E(0^+)$: $E(0^-) = \dfrac{qN_D}{K_n\varepsilon_0}x_n = \boxed{3.27 \times 10^7\text{ V/m}}$

$$E(0^+) = \frac{qN_A}{K_p\varepsilon_0}x_p = \boxed{2.92 \times 10^7\text{ V/m}}$$

Finally, $V_{JN} = -V(0) = +\dfrac{qN_D x_n^2}{2K_N\varepsilon_0} = \boxed{1.59\text{ V drop from } x = -\infty}$, $V_{JP} = V(0) + V_{BI} = \dfrac{qN_A x_p^2}{2K_p\varepsilon_0} = \boxed{28.4\text{ meV drop}}$

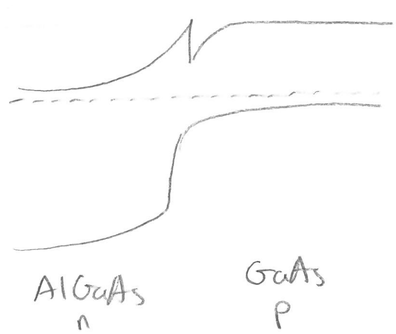
6. If the 2 parts are uniformly n-doped, then $\delta_1 \approx \delta_2$, so when the graded structure is put together the fermi levels will equalize and the conduction band will be flat while the valence band has a linear slope. This will look like:



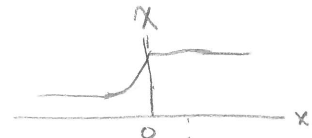


I did quadratic grading first, by accident. Linear is next.

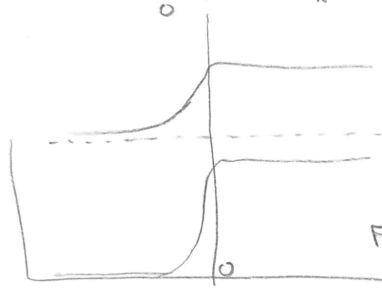
b. 9. The band diagram, after creating the junction, will look like



But we can get rid of the spike by grading if the diagram of $\chi(x)$ looks like:

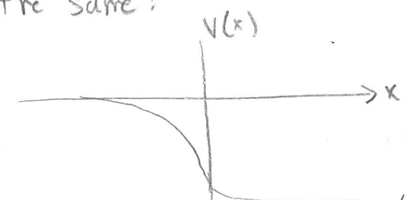


, then the raw band diagram we become:



The spike will be smoothed, and if the grading is quadratic it will become abruptly flat.

In all cases, V(x) will be the same:



and most of V will drop on the n side.

Then to get the band diagrams we add $-\chi(x)$ to $-V(x)$ (to get $E_c(x)$). To exactly cancel out the spike, then $\chi(x)$ at the junction should change in the same but opposite way to how $V(x)$ is changing. As $N_A \gg N_D$, we can approximate $V(x) = V_{BI}\left(1-\left(1+\frac{x}{x_n}\right)^2\right)$ on the n side,

$\chi(x) = \chi_{GaAs} - \Delta\chi(x)$, generally, so exactly canceling means $\Delta\chi(x) = qV(x) = qV_{BI}\left(1-\left(1+\frac{x}{x_n}\right)^2\right)$

Finally, we are restricted to $\chi(x_g) = \chi_{AlGaAs} \Rightarrow \Delta\chi(x_g) = \Delta E_c$, so at the end of the grading $\Delta E_c = qV_{BI}\left(1-\left(1+\frac{x_g}{x_n}\right)^2\right) \Rightarrow x_g = x_n\left(1-\sqrt{1-\frac{\Delta E_c}{qV_{BI}}}\right) = \boxed{7.18 \text{ nm}}$

The band diagram in equilibrium is above

When a forward bias is applied, the builtin potential will effectively be lower, so the grading width will no longer be enough to compensate, and the spike will reappear. The size of the spike will be smaller, though, because it is partially compensated.

A simulated band diagram with 7.2 nm quadratic grading is attached, and indeed the spike is all but fully removed.

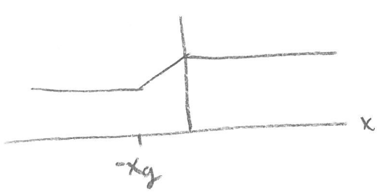
8. Now, with a linear grading, the compensation will not be as perfect, but we can still fix it somewhat.

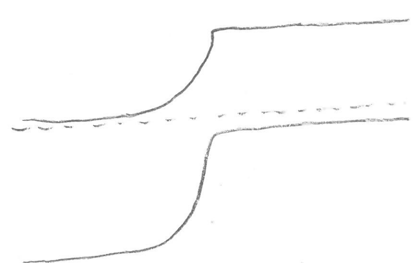
This time, the criteria is that the electric field created by the linear grading should be equal to the electric field created by the depletion region.

The field created by the depletion region is at most $-\frac{dV}{dx}\Big|_{x=0^-} = E(0^-)$, and the field created by the grading has magnitude $\frac{\Delta E_c / q}{x_g}$, so $\frac{\Delta E_c}{q x_g} = E(0^-)$

$$\Rightarrow x_g = \frac{\Delta E_c}{q E(0^-)} = \boxed{7.04 \text{ nm}}$$

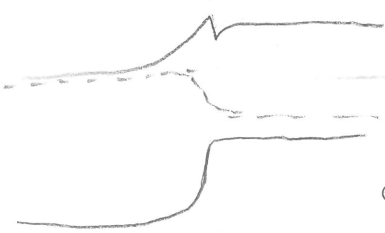
Now $\chi(x)$ looks like: so the band diagram will look like





where there should be a sharper corner because we overcompensated due to the wrong form.

With a forward bias of 1.2 V, the effective V_{BI} will be smaller so $E(0^-)$ will be smaller and x_g will no longer be big enough to remove the spike. This will look like:



This time the spike may be slightly more pronounced because the linear grading is imperfect.

A simulated band structure is again attached. It is very similar to the quadratic grading case, except the spike is a little more pronounced.

Sorry for the printing quality, the printer available had some problem.

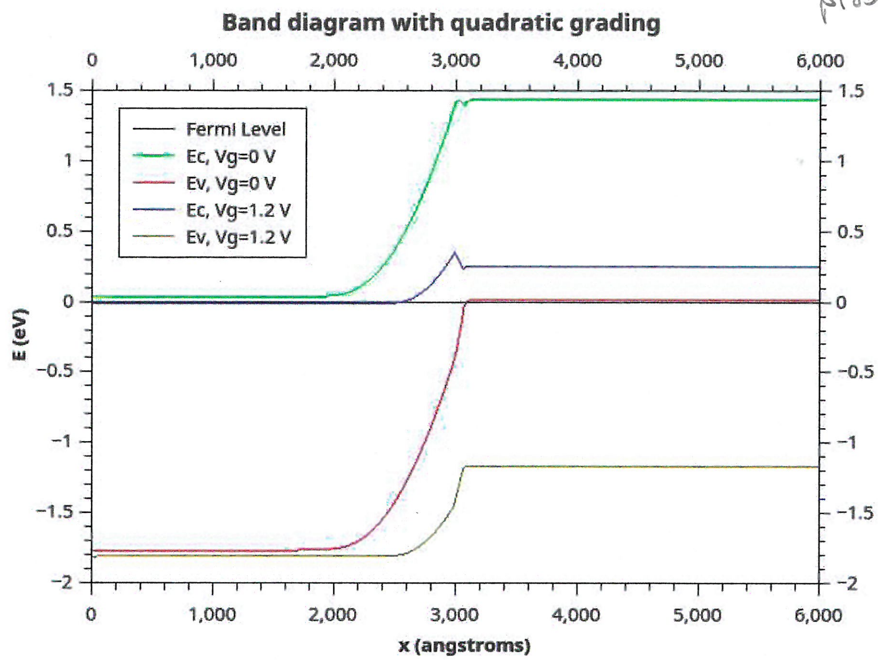


Figure 1: Band diagram corresponding to problem 9, using quadratic grading to remove the spike. The band diagram is shown for no gate bias and 1.2 V forward bias.

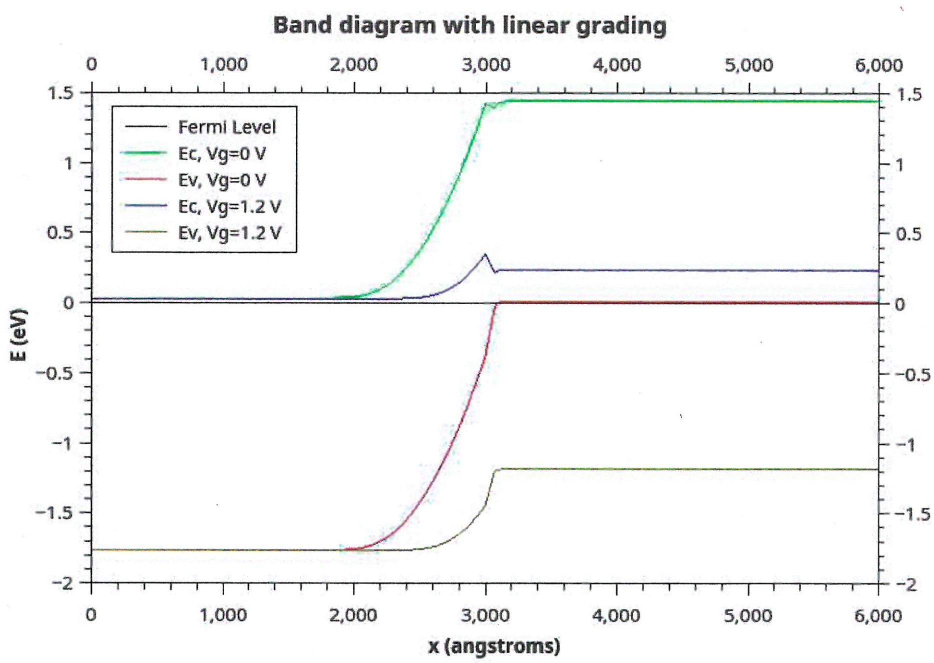
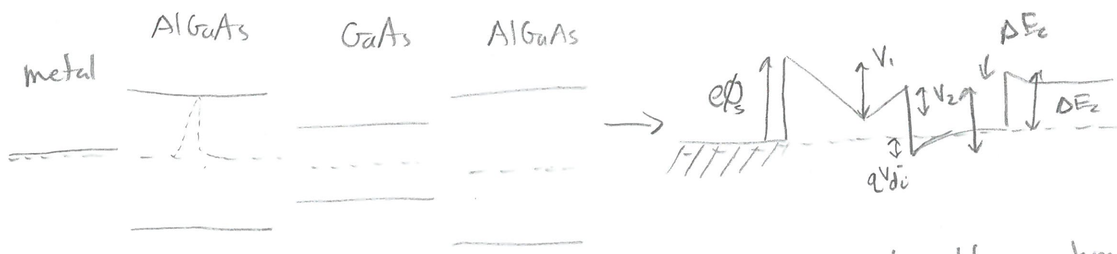
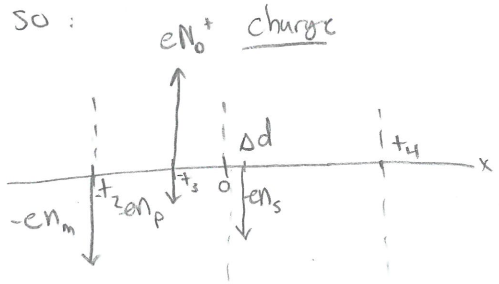


Figure 2: Band diagram corresponding to problem 8, using a linear grading to remove the spike. The band diagram is shown for no gate bias and 1.2 V forward bias.

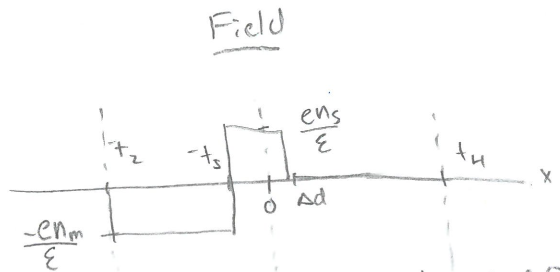
3.2) a. To find the QW sheet density, we will start with the approximate band diagram:



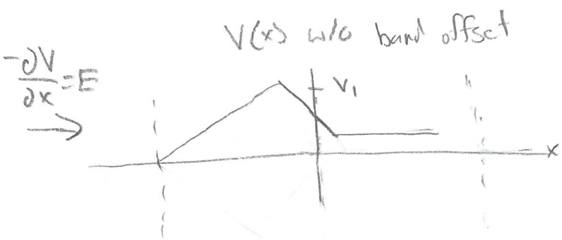
From this, we can see that the charges put into the system get distributed into the quantum well, the metal / AlGaAs interface and some stay at the doping site, so:



$\frac{\partial E}{\partial x} = \frac{\rho}{\varepsilon}$



$-\frac{\partial V}{\partial x} = E$



To solve this, we approximate $n_p \approx 0$, then assert ① charge conservation
② energy conservation

① $N_D^+ = n_m + n_s$

② (following the band structure) $\phi_s - V_1 + V_2 - \Delta E_c/e + V_{di} = 0$ → this means all the local wirdness cancels out at the edges and $V(0) = V(\text{end}) = 0$

$V_1 = \frac{+en_m}{\varepsilon}(t_2 - t_3)$, $V_2 = \frac{en_s}{\varepsilon}(t_3)$, by integrating the field.

$V_{di} = \frac{\pi\hbar^2}{m^*} n_s$ = voltage drop across the quantum well. $\Delta d = \frac{\varepsilon\pi\hbar^2}{em^*}$, so $V_{di} = \Delta d \frac{e}{\varepsilon} n_s$

②'

so: $\phi_s - \frac{en_m}{\varepsilon}(t_2 - t_3) + \frac{en_s}{\varepsilon} t_3 - \frac{\Delta E_c}{e} + \frac{\Delta d\, e\, n_s}{\varepsilon} = 0$

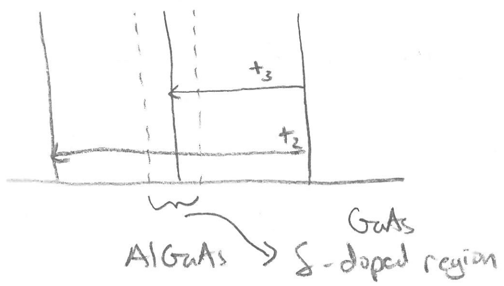
Two variables (n_s, n_m), two equations → $\boxed{n_s = \frac{eN_D^+(t_2 - t_3) + \varepsilon(-\phi_s + \Delta E_c/e)}{e(t_2 + \Delta d)}}$

Technically, ε changes from GaAs to AlGaAs, but they are both $\sim 12.5\,\varepsilon_0$, so that is the value I will use.

Plugging in the #s: $\boxed{n_s = 7.65 \times 10^{11}\ \text{cm}^{-2}}$ The value used for Δd came from the simulated solution, specifically I chose it to correspond to the charge density in the simulation, the maximum in charge density. While this required three use of the simulation, there is no way to guess analytically. The value was 4.5 nm.

one can guess Δd based on quantum capacitance.

Using these same values, the self-consistant simulation gave $\boxed{n_s = 5.36 \times 10^{11}\ cm^{-2}}$, which is pretty close, but not perfect. The error probably comes from the inability to get true δ-doping. To get this, I put the 1 nm δ-doping region half on the left and half on the right.

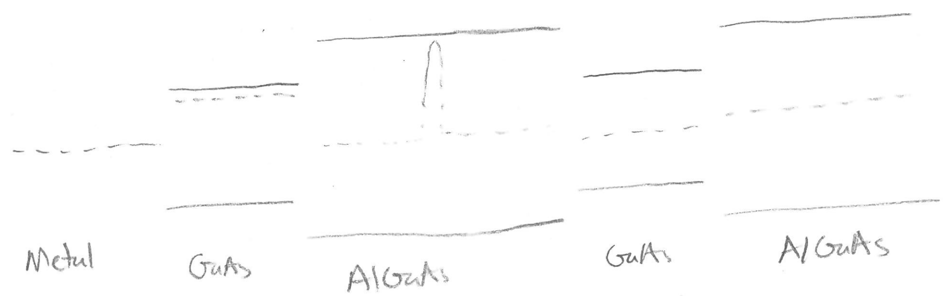


The simulation also gives 3 confined states, with energies 2.38 meV below E_F
160 meV above E_F
168 meV above E_F

The plot of the simulated band structure is attached.

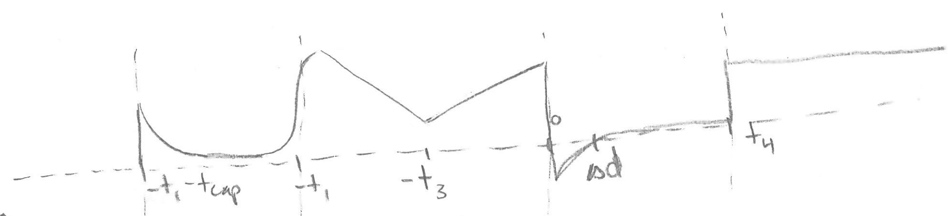
Note: When doing all of this, I had to include a 300 nm thick $Al_{0.3}Ga_{0.7}As$ region behind the GaAs, to act as the semi-insulating AlGaAs.

b. Near the S/D regions, the band structure will look like

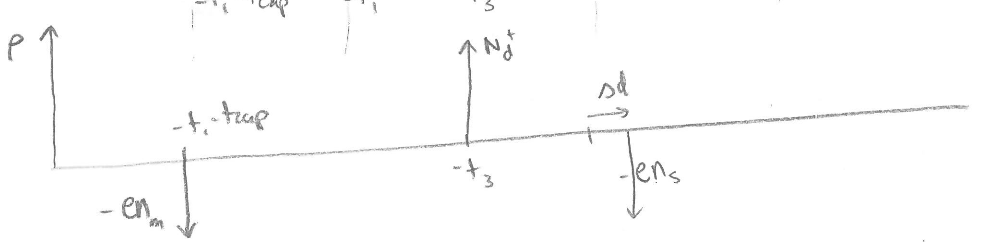


before creation

after creation

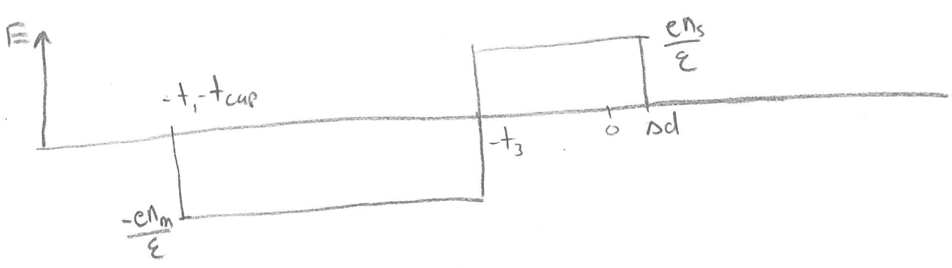


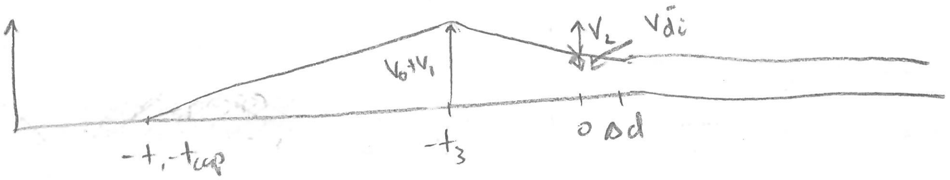
Again there will be doping charge, and free sheet charge at the metal interface and in the quantum well:



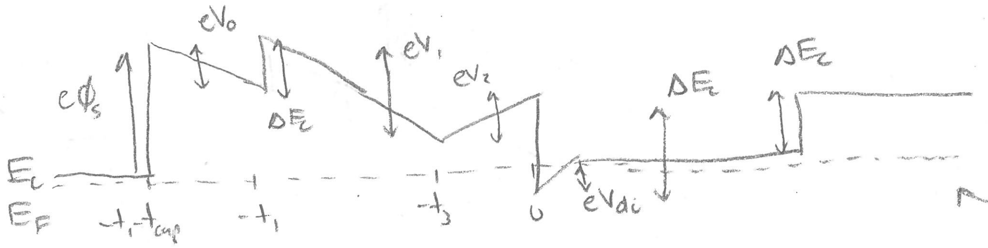
Almost all the same electrostatics applies:

$$\frac{\partial E}{\partial x} = \frac{\rho}{\varepsilon}, \quad -\frac{\partial V}{\partial x} = E$$





Now when we add $-V(x)$ to $-\chi(x)$, we can see what $E_c(x)$ will actually look like:



So in reality, the band diagram is a little different from what was initially thought, but this should be more accurate.

Quantitatively, everything is the same as before, except that ② becomes

$$\phi_s - V_0 + \frac{\Delta E_c}{e} - V_1 + V_2 - \frac{\Delta E_c}{e} + V_{di} = 0, \quad V_{di} = \Delta d\, n_s \frac{e}{\varepsilon}$$

$$V_0 + V_1 = \frac{+en_m}{\varepsilon}(t_1 + t_{cap} - t_3), \quad V_2 = \frac{en_s t_3}{\varepsilon}, \quad \text{so:}$$

$$\phi_s - \frac{e(N_D^+ - n_s)}{\varepsilon}(t_1 + t_{cap} - t_3) + \frac{en_s t_3}{\varepsilon} + \Delta d\, n_s \frac{e}{\varepsilon} = 0$$

$$\Rightarrow n_s = \frac{\left(\frac{eN_D^+}{\varepsilon}(t_1 + t_{cap} - t_3) - \phi_s\right)\frac{\varepsilon}{e}}{\Delta d + t_1 + t_{cap}} = \boxed{\frac{eN_D^+(t_1 + t_{cap} - t_3) - \varepsilon\phi_s}{e(t_1 + t_{cap} + \Delta d)}}$$

Putting in the #s, again using $\varepsilon = 12.5\varepsilon_0$, I get $\boxed{n_s = 1.34 \times 10^{12}\ cm^{-2}}$

The simulation gives $\boxed{n_s = 1.07 \times 10^{12}\ cm^{-2}}$, which is fairly close. Actually, it is within the error in ε, so at this point that is probably the largest error from the simulations.

Again I use 4.5 nm for Δd, which comes from the simulations.

A plot of the simulated band structure is attached.

This time, the Fermi level is a little higher in the well, so the eigenstates are at:

31.4 meV below E_F 183 meV above E_F
67.7 meV above E_F 187 meV above E_F
137 meV above E_F 204 meV above E_F

Still only 1 subband is filled ($E < E_F$), but the quantum confinement is significant.

c. To first order, this geometry is a capacitor: the gate is coupled capacitavely to the 2DEG without being able to directly flow current. The capacitance is just that of a parallel plate capacitor:

$$C_g = \text{Capacitance per area} = \frac{\varepsilon}{dist} = \boxed{\frac{\varepsilon}{t_2 + \Delta d}}$$

Here, with $\varepsilon = 12.5\varepsilon_0$ and $\Delta d = 4.5$ nm

$$C_g = 5.14 \times 10^{-3}\ F/m^2 = \boxed{515\ nF/cm^2}$$

A plot of C_g vs. V_g as calculated by the program is attached. At $V_g = 0V$, $C_g = 430\ nF/cm^2$, which is close, but lower than the analytical value. As $|V_g|$ increases, C_g decreases, which is not captured at all in the simple analytical approximation that the setup acts like a parallel plate capacitor.

d. The threshold voltage, V_{TH}, is the voltage when $n_s = 0$.

Including V_G, $n_s = \dfrac{eN_d^+(t_2 - t_3) + \varepsilon(V_G - \phi_s + \Delta E_c/e)}{e(t_2 + \Delta d)}$, So solving $n_s = 0$

$$\Rightarrow V_G = \frac{-eN_d^+(t_2 - t_3)}{\varepsilon} + \phi_s - \Delta E_c/e = \boxed{V_{TH} = -0.238\text{ V}}$$

To verify this with the simulation, I ran the simulation with V_G values from 0 V to -0.4 V, at -0.02 V intervals. Plots of n_s vs. V_G in both linear scale and log scale are attached. In the linear scale plot, it's apparent that for small V_G, n_s is linear in V_G, just as our model predicts. At larger V_G, however, as the gate pushes the QW away from E_F, n_s becomes exponential in V_G, which is what would be expected just from $n = N_c e^{-(E_c - E_F)/kT}$. We can confirm the decay is exactly exponential in the log scale plot, where for $V_G \lesssim -0.24$ the line appears straight.

Finally, to calculate V_{TH}, the linear region has been extrapolated to where it would intersect 0 sheet charge. This gives $\boxed{V_{TH} \approx -0.22\text{ V}}$, which is fairly close to the analytical calculation.

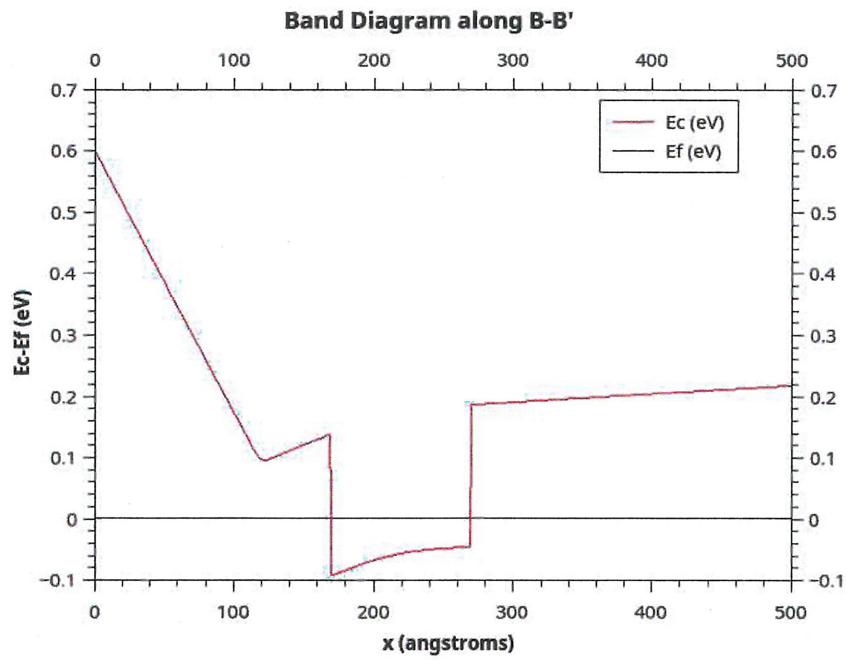


Figure 1: Band diagram of the AlGaAs/GaAs HEMT along the B-B' line.

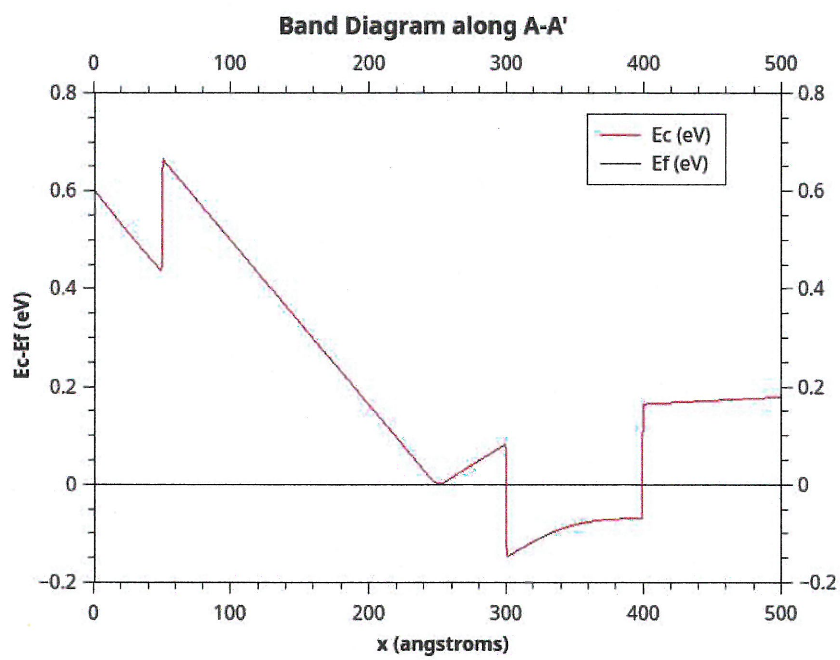


Figure 2: Band diagram of the GaAs capped AlGaAs HEMT along the A-A' line.

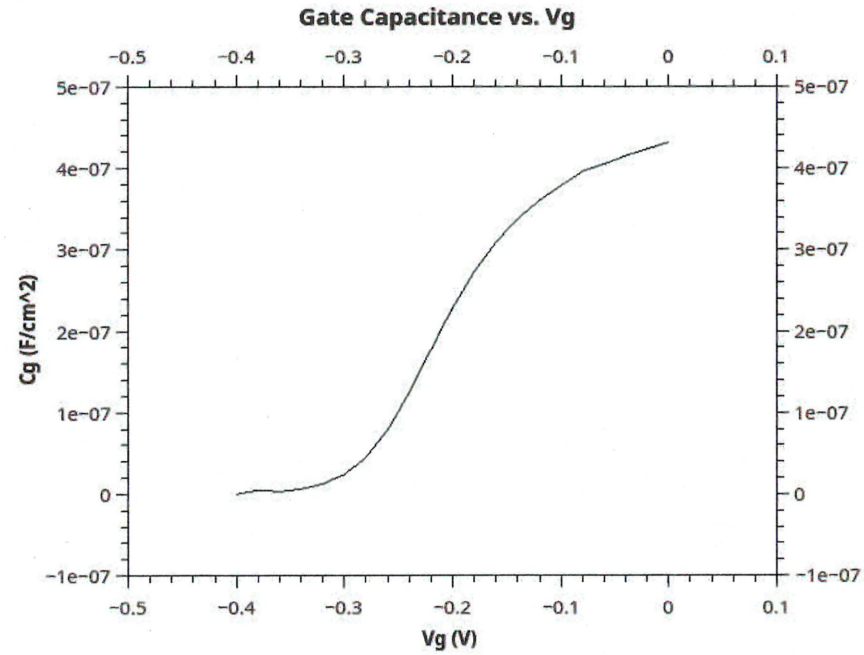


Figure 3: Gate capacitance vs. applied gate voltage for the HEMT.

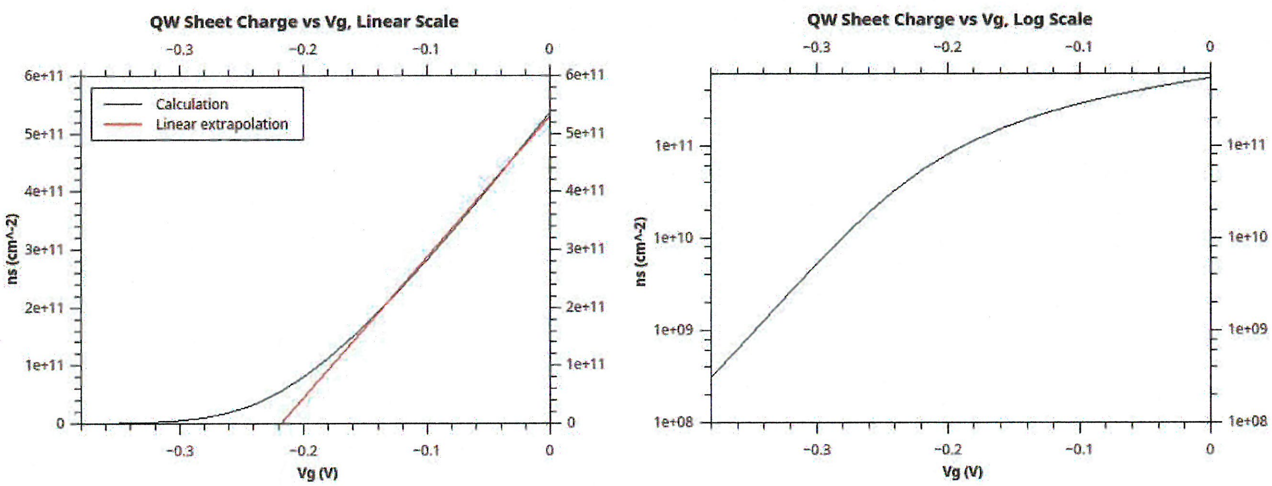


Figure 4: Sheet charge in the quantum well vs. applied gate voltage, in both linear and log scale.

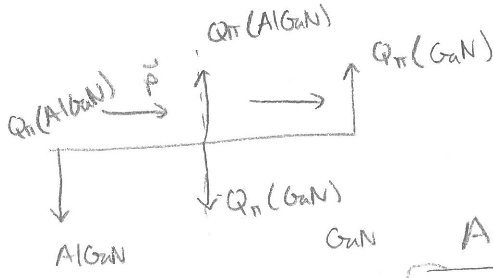
3.3) a.

In the $Al_xGa_{1-x}N$ there is polarization from both spontanious polarization, and from strain.
In the GaN, there is only spontanious polarization.

For GaN: $P_{sp} = -0.034 \frac{C}{m^2} = Q_\pi \text{ (GaAs)}$

For $Al_xGa_{1-x}N$: $\left.\begin{aligned} P_{sp} &= -0.034 - 0.035x - 0.021x^2 \frac{C}{m^2} \\ P_{pz} &= -0.0243x - 0.0292x^2 \frac{C}{m^2} \end{aligned}\right\} Q_\pi \text{(AlGaAs)}$

So this is like



So right at the junction

these are both negative

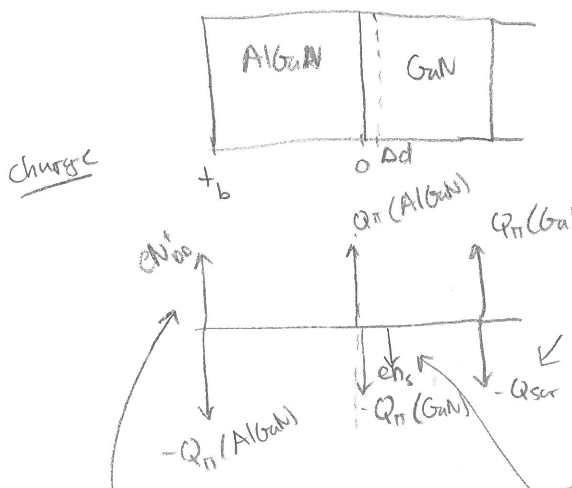
$Q_\pi(\text{net}) = Q_\pi(\text{GaN}) - Q_\pi(\text{AlGaN})$

$= \boxed{0.0593x + 0.0492x^2 \frac{C}{m^2}}$

At $x = 0.3$, $Q_\pi(\text{net}) = 0.0222 \frac{C}{m^2}$, so

$\boxed{n = \frac{Q_\pi}{q} = 1.39 \times 10^{13} \text{ cm}^{-2}}$

b. At a junction like this, what really happens is



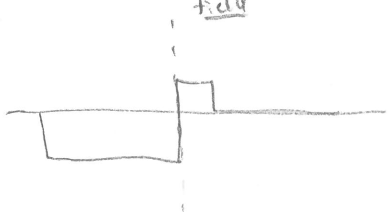
These come from screening charges near the substrate, that cancel out the Q_π from GaN there

These come from deep donor states at the surface, and partially reduce the effect of the band bending in AlGaN

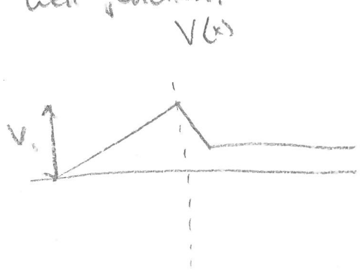
This is the mobile sheet carrier density at the quantum well junction.

Using $\frac{\partial E}{\partial x} = \frac{\rho}{\varepsilon}$

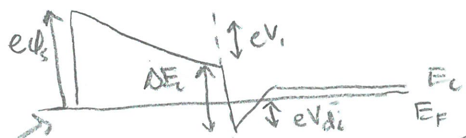
field



using $\frac{\partial V}{\partial x} = -E \rightarrow$



This creates a band structure: (flip $V(x)$, add $X(x)$)



In this we technically have 2 unknowns, n_s and N'_{DD}. We can write everything in terms of n_s, though:

① Energy conservation (following the band structure)

$\phi_s - V_1 - \frac{\Delta E_c}{e} + V_{di}^{-} = 0$, where V_{di} = voltage drop in quantum well $= \frac{\pi\hbar^2}{m^*} n_s = \frac{\Delta d\, e}{\varepsilon} n_s$

also $V_1 = \frac{\left[eN'_{DD} - Q_\pi(AlGaN)\right] t_b}{\varepsilon}$, but by ② Charge conservation:

$$\underbrace{eN'_{DD} - Q_\pi(AlGaN) + \underbrace{Q_\pi(GaN) - Q_{scr}}_{\text{exactly cancel}}}_{} = \underbrace{Q_\pi(net) - en_s}_{\text{junction total charge}}$$

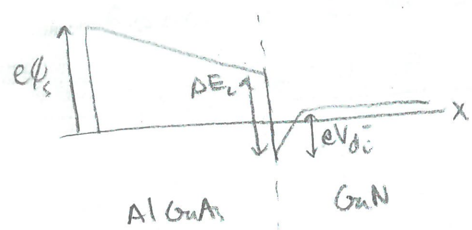
so $V_1 = \frac{(Q_\pi(net) - en_s)\, t_b}{\varepsilon}$

plugging this in gives $\phi_s - \frac{Q_\pi(net)\, t_b}{\varepsilon} + \frac{en_s t_b}{\varepsilon} - \frac{\Delta E_c}{e} + \frac{\Delta d\, e}{\varepsilon} n_s = 0$

$$\Rightarrow n_s = \frac{\varepsilon}{e}\left(\frac{Q_\pi(net)\, t_b}{\varepsilon} - \phi_s + \Delta E_c/e\right)\frac{1}{(t_b + \Delta d)} = \boxed{\frac{Q_\pi(net)\, t_b + \varepsilon(-\phi_s + \Delta E_c/e)}{eD}}, \quad D = t_b + \Delta d$$

A plot of this is attached, as a function of t_b.

c. Just like before, the band diagram will look like:

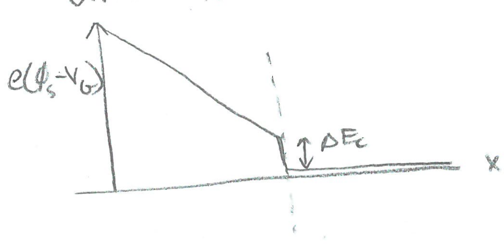


at 0 gate bais. When there is a gate votage applied, the only difference is ϕ_s will become $\phi_s - V_G$, so

$$n_s = \frac{Q_\pi(net)\, t_b + \varepsilon\left(V_G - (\phi_s - \Delta E_c/e)\right)}{eD}$$

Pinch off happens when $n_s = 0 \Rightarrow V_G = -\frac{Q_\pi(net)\, t_b}{\varepsilon} + \phi_s - \frac{\Delta E_c}{e}$ $= \boxed{-7.33\ V}$

At pinch off, the gate will push up the barrier height until there is no more quantum well to confine electrons:

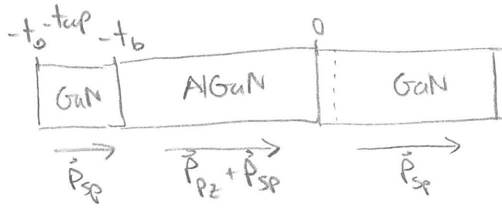


Note: I used a 400 nm GaN substrate in simulations.

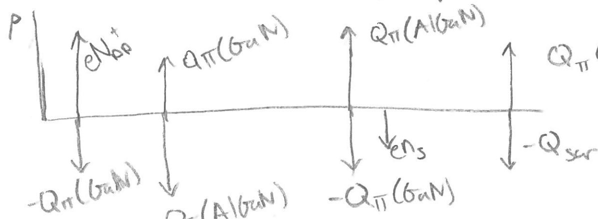
The simulation gives slightly different results: plots of the band diagrams at $V_g = 0$ and $V_g = -7.0$ V are attached. When $V_g = 0$, everything looks the same, but when $V_g = -7$ V, we can see that instead of continuing forever, a neutralizing dipole is not real formed once V_g bends the bands enough. This prevents the bands from continuing to bend, and does not lift the QW above E_F. This way, the V_{TH} condition $n_s = 0$ is never reached. To get an estimate for what it would be, a plot of n_s vs. V_G is attached, showing a linear extrapolation from the linear region. It intersects 0 at ~ −8.5 V, which is close but not exactly the analytical value.

need to set E_F manually

d. This geometry is very similar to the one without the cap, except there is another set of polarization charges:

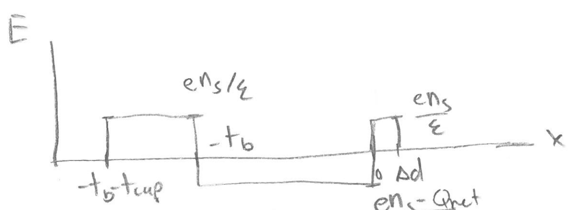


This will create a charge profile like:

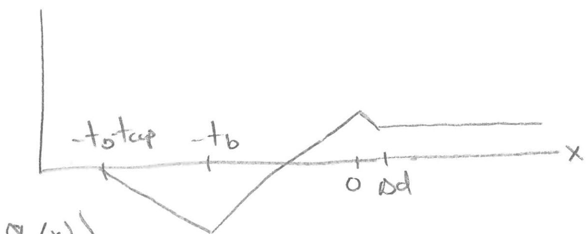


it's hard to know for sure what $N_{DD}^+ - Q_\pi(GaN)$ will be, but it turns out to be positive. At the other interfaces, we know for sure that $Q_\pi(AlGaN) - Q_\pi(GaN) = Q_\pi(net)$, which is the same as before.

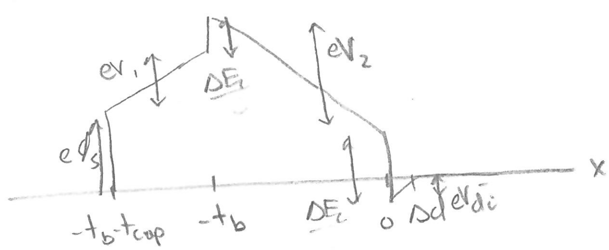
To get E: $\frac{\partial E}{\partial x} = \frac{\rho}{\varepsilon}$:



$\frac{\partial V}{\partial x} = -E$ $\longrightarrow$



This creates a band structure like: $(-V(x) - \chi(x))$



We need to find V_{TH}, so we need to solve for n_s again:

① Charge conservation:

$$eN_{DD}^+ - Q_\pi(GaN) = en_s$$

① Energy conservation:

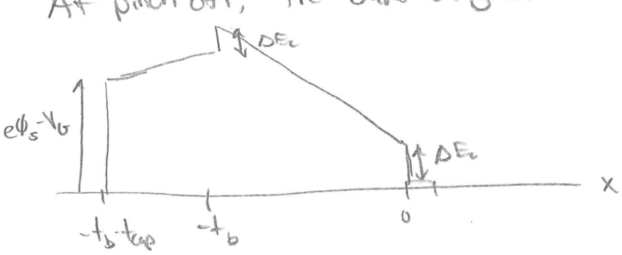
$$-V_g + \phi_s + V_1 + \Delta E_c/e - V_2 - \Delta E_c/e + V_{di} = 0, \quad \text{with } V_{di} = \frac{\Delta d\, e}{\varepsilon} n_s$$

$$V_1 = \frac{(eN_{DD}^+ - Q_\pi(GaN))}{\varepsilon} t_{cap}, \quad V_2 = -\frac{(en_s - Q_\pi(net))}{\varepsilon} t_b, \quad \text{so: (using ① into ②)}$$

$$-V_G + \phi_s + \frac{en_s t_{cap}}{\varepsilon} + \frac{en_s t_b}{\varepsilon} - \frac{Q_\pi(net) t_b}{\varepsilon} + \frac{\Delta d\, e n_s}{\varepsilon} = 0$$

$$\Rightarrow \boxed{n_s = \frac{Q_\pi(net) t_b + \varepsilon(V_G - \phi_s)}{e(t_{cap} + t_b + \Delta d)}} \qquad V_{TH} = V_G(n_s = 0) = \boxed{\frac{-Q_\pi(net) t_b}{\varepsilon} + \phi_s} = \boxed{-7.46\text{ V}}$$

At pinch off, the band diagram should look like: (not the same scale)

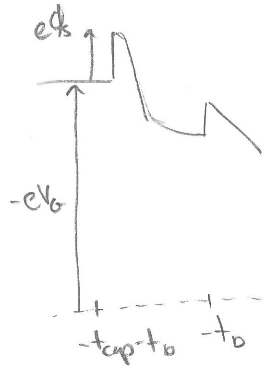


The results of the simulation are similar to last time: in reality a neutralizing dipole forms and so n_s is never really 0. The plot of the band structure at $V_G = 0$, and $V_G = -4$V is attached.

At $V_G=0$, the effective Schottky barrier height is $e\phi_s + eV_1 + \Delta E_c$, because that is the potential an electron in the metal needs to overcome to make it into the 2DEG.

This value is $e\phi_s + \Delta E_c + \frac{e^2 n_s t_{cap}}{\varepsilon} = \boxed{2.52\text{ eV}}$

At pinch off, because of the neutralizing dipole that forms in reality (see plot at $V_G=-4V$) the band diagram near the metal looks like:



So in this case the effective Schottky barrier is just the real Schottky barrier, $\boxed{0.9\text{ eV}}$

For comparison, the effective Schottky barrier without the cap is 1.7 eV. As a higher barrier means less gate leakage, this means that the GaN-capped geometry should have less gate leakage, at least for relatively small V_G where the neutralizing dipole has not formed yet.

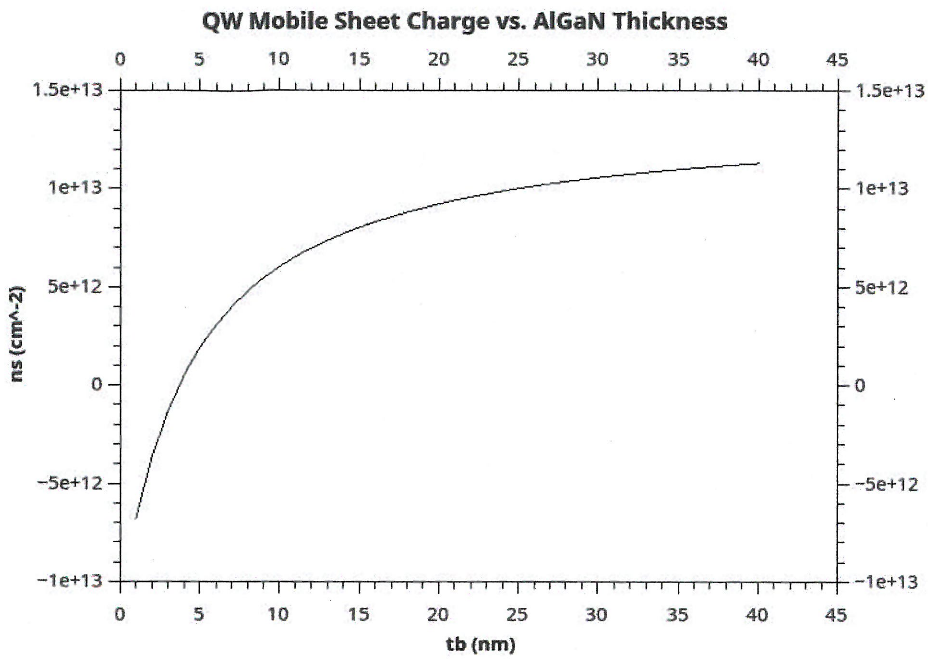


Figure 1: Quantum well sheet charge vs AlGaN thickness.

Need to set Ef manually ; to avoid this

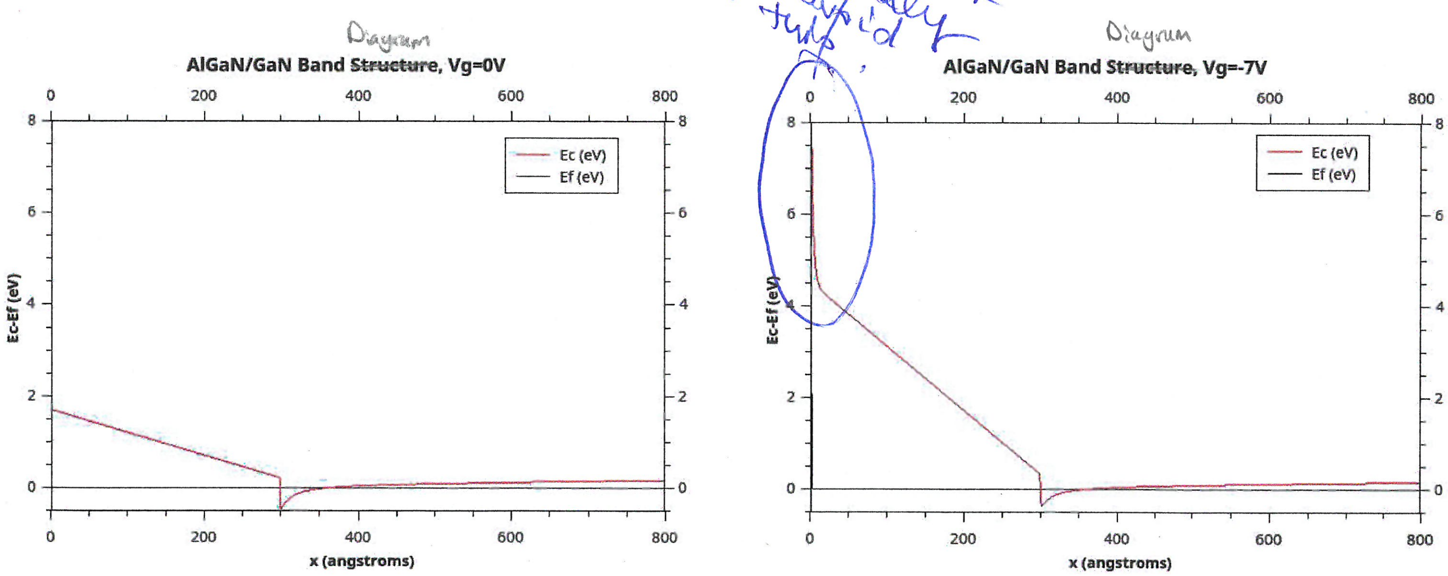


Figure 2: AlGaN/GaN band diagram for 0 gate voltage and near pinch off. Instead of reducing the sheet charge density as in the calculation, the formation of a neutralizing dipole mitigated the effect of the gate bias.

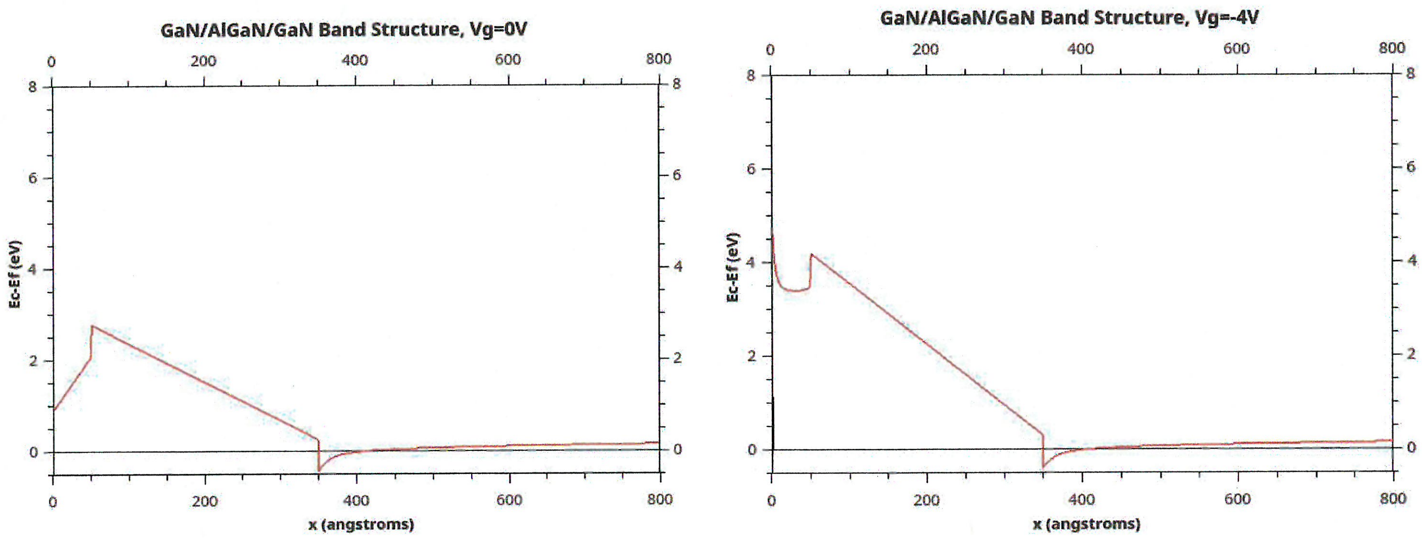


Figure 3: GaN/AlGaN/GaN band diagram for zero gate bias and approaching pinch off. Pinch off was calculated to occur near -7.5 V, but the same neutralizing dipole effect occurs so the band diagram was plotted at -4V instead, near where the gate bias begins to be unable to modulate the sheet charge density.

3.4) a. In general, $\alpha_0(\hbar\omega) = C_0 |\hat{e}\cdot\vec{p}_{cv}|^2 \rho_r(\hbar\omega - E_g)$, where

$C_0 = \frac{\pi e^2}{n_r c \varepsilon_0 m_0^2 \omega}$, $|\hat{e}\cdot\vec{p}_{cv}|^2$ is the momentum matrix element, and ρ_r is the joint density of states.

For all the following calculations I used:

n_r = index of refraction of GaN = 2.3
$E_g = 3.4$ eV
$m_e^* = 0.2\, m_0$
$m_h^* = 1.4\, m_0$

Also I assumed Δ was small, so that $|\hat{e}\cdot\vec{p}_{cv}|^2 = \left(\frac{m_0}{m_e^*} - 1\right)\frac{m_0 E_g}{6}$. This seems to be a decent approximation, although it may be ~10% off.

Finally $\rho_r(\hbar\omega - E_g) = \text{JDOS} = \frac{g_s g_v}{(2\pi)^2}\left(\frac{2m_r^*}{\hbar^2}\right)^{3/2}\sqrt{\hbar\omega - E_g}$, where $m_r^* = \left[\frac{1}{m_h^*} + \frac{1}{m_e^*}\right]^{-1}$

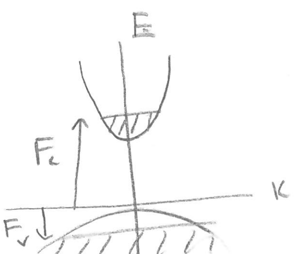
I also used $g_v = 1$, $g_s = 2$.

This leads to the plot of $\alpha_0(\hbar\omega)$ attached. Qualitatively it looks correct, with the coefficient being 0 for $\hbar\omega < E_g$, and $\alpha_0 \propto \frac{\sqrt{\hbar\omega - E_g}}{\hbar\omega}$ for $\hbar\omega > E_g$, of course. Qualitatively it looks plausable, as $\alpha_0 \sim 10000\ \text{cm}^{-1}$.

b. To get the true, non-equilibrium absorbtion coefficient, we need to include the occupation functions $f_c(\vec{k})$ and $f_v(\vec{k})$:

$$f_c(\vec{k}) = \frac{1}{1 + e^{(E_c(\vec{k}) - F_c)/kT}} \qquad f_v(\vec{k}) = \frac{1}{1 + e^{(E_v(\vec{k}) - F_v)/kT}}$$

where F_c and F_v are defined as the quasi-Fermi energies for the conduction band and the valence band.



Given that $F_c - F_v = E_g + 0.2$ eV, I made each F_c and F_v take half of the change, i.e. $\boxed{F_c = E_g + 0.1\ \text{eV}}$ and $\boxed{F_v = -0.1\ \text{eV}}$. This choice was arbitrary, but it should not make a large difference on the final result.

With this, then, I have plotted $f_v(k_0) - f_c(k_0)$ (see attached) where $k_0 = \sqrt{\frac{2m_r^*}{\hbar^2}(\hbar\omega - E_g)}$. The shape can be explained as follows:

For $\hbar\omega$ right at E_g (or less), $f_c \sim 1$ and $f_v \sim 0$, so emittion at $\hbar\omega$ is likely $\Rightarrow f_v - f_c = -1$. As f_c gets smaller and f_v gets larger with larger $\hbar\omega$, eventually $f_v \sim 1$ and $f_c \sim 0$, so population inversion is no longer the case and normal absorption occurs $\Rightarrow f_v - f_c = 1$.

c. The net absorption coefficient $\alpha(\hbar\omega)$ is attached. It was calculated as $\alpha(\hbar\omega) = \alpha_0(\hbar\omega)[f_v(k_0) - f_c(k_0)]$. It shows a small region of gain right after $\hbar\omega = E_{\overline{G}}$, followed by a return to absorbance.

d. The gain spectrum is also attached. This is just $-\alpha(\hbar\omega)$, for $\hbar\omega$ near $E_{\overline{G}} = 3.4$ eV.

From this plot, the maximum gain occurs at $\boxed{3.47 \text{ eV}}$, with a value of $\boxed{6500 \text{ cm}^{-1}}$.

First, I found in "Optical Gain of Strained Wurtzite GaN Quantum-Well Lasers" L. Chuang, IEEE J. Quantum electronics, the results of more sophisticated calculations. This gives $\boxed{\sim 7000 \text{ cm}^{-1} \text{ at } 3.62 \text{ eV}}$ for $L_w = 2.6$ nm and $\boxed{\sim 4100 \text{ cm}^{-1} \text{ at } 3.54 \text{ eV}}$ for $L_w = 5$ nm.

So it seems like as the QW is squeezed, the effective band gap increases because of quantization of the energies. At the same time, a narrow well allows for the population inversion $F_c - F_v - E_{\overline{G}} = 0.2$ eV, so the wider the well the smaller the gain.

Second, in "Large optical gain AlGaN-delta-GaN quantum wells laser active regions in mid- and deep-ultraviolet spectral regimes," Zhang et al., APL 2011, I found some experimental results. They mainly care about very narrow wells, and report $\boxed{g = 4500 \text{ cm}^{-1} \text{ at } 4.9 \text{ eV}}$ with a 3Å well. So the gain is close to my simple calculation, but because the well is so narrow the energy is pushed up quite a bit. They also show results for wider wells, giving $\boxed{g = 500 \text{ cm}^{-1} \text{ at } 3.5 \text{ eV}}$ for a 2.7 nm well. Now with the wider well population inversion is harder, and the gain is smaller than my calculations.

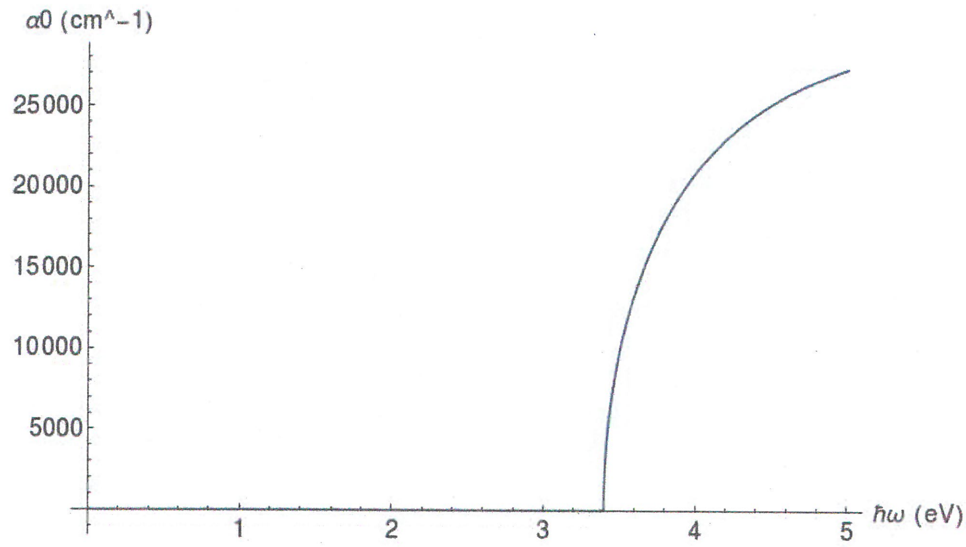


Figure 1: Equilibrium absorption coefficient as a function of photon energy.

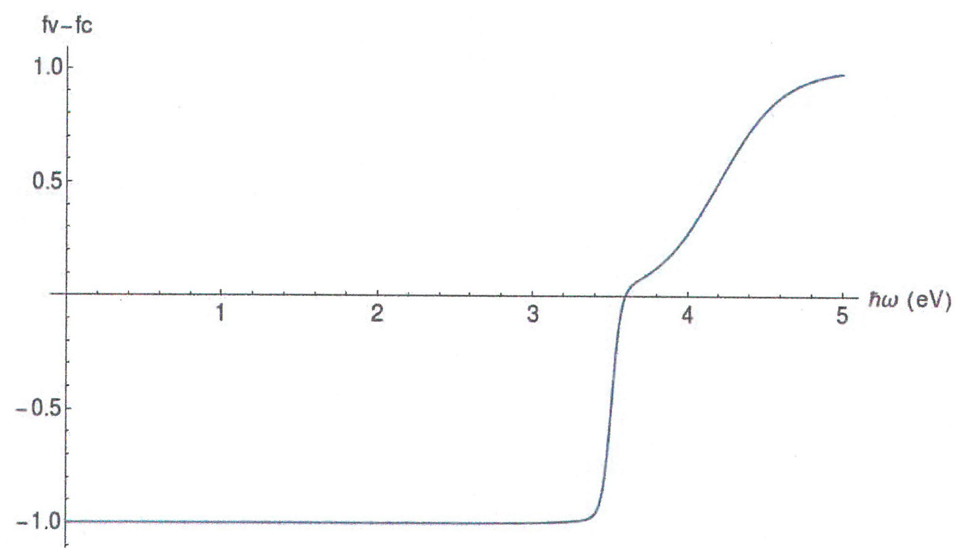


Figure 2: Combined occupation function fv(k0) – fc(k0) as a function of photon energy.

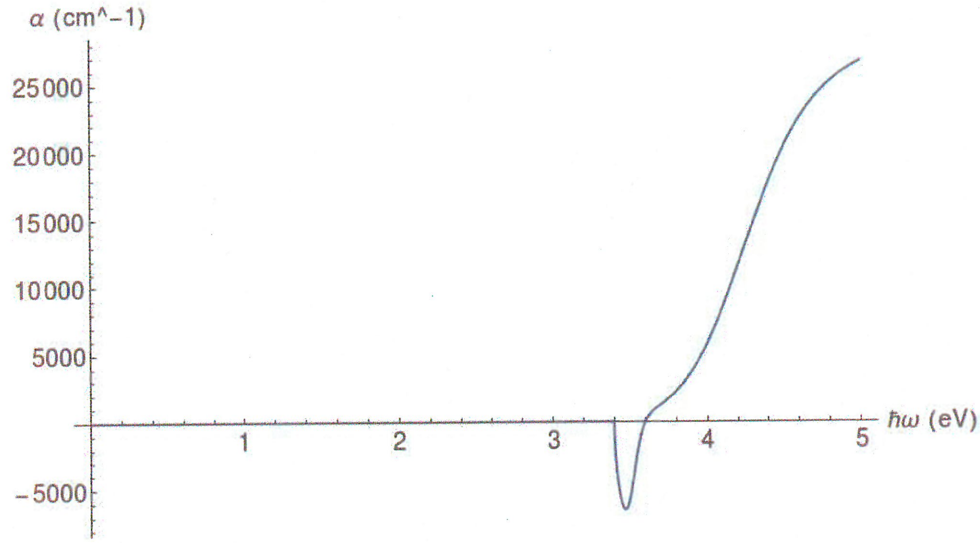


Figure 3: Total out-of-equilibrium absorption coefficient as a function of photon energy.

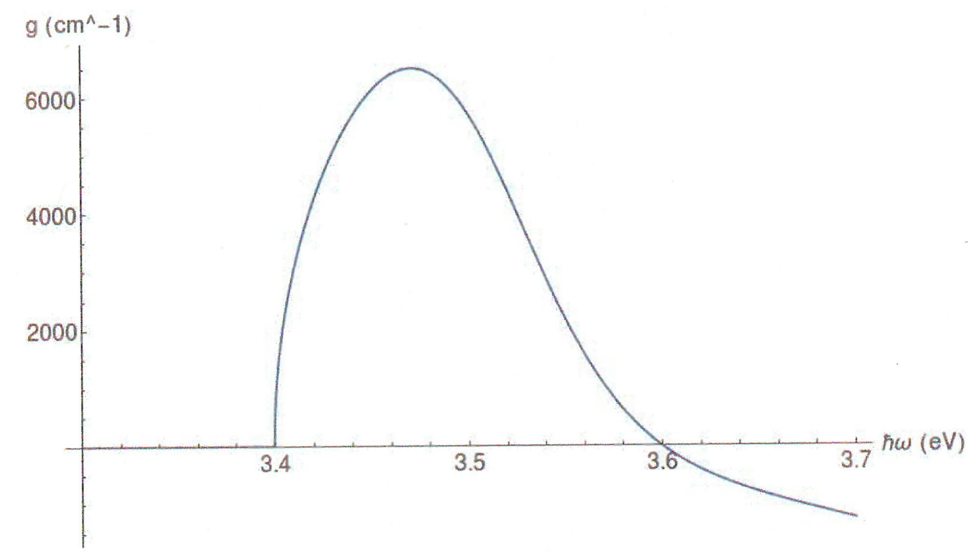


Figure 4: Calculated gain spectrum of GaN, for the range of photon energies where gain is positive.